

Generation of Fractional Factorial Designs

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Abstract

The joint use of counting functions, Hilbert basis and Markov basis allows to define a procedure to generate all the fractions that satisfy a given set of constraints in terms of orthogonality. The general case of mixed level designs, without restrictions on the number of levels of each factor (like primes or power of primes) is studied. This new methodology has been experimented on some significant classes of fractional factorial designs, including mixed level orthogonal arrays.

Key words: Design of Experiments, Hilbert basis, Markov basis, Algebraic statistics, Indicator polynomial, Counting function.

1 Introduction

All the fractional factorial designs that satisfy a set of conditions in terms of orthogonality between factors have been described as the zero-set of a system of polynomial equations in which the indeterminates are the complex coefficients of their counting polynomial functions (Pistone and Rogantin (2008), Fontana et al. (2000)). A short review of this theory can be found in Fontana and Rogantin (2008). In Section 2 we report a part of it to facilitate the reader. In Section 3 we write the problem of finding fractional factorial designs that satisfy a set of conditions as a system of linear equations in which the indeterminates are positive integers. In section 4, using 4ti2 (4ti2 team (2007)) we find all the generators of some classes of fractional factorial designs, including mixed level orthogonal arrays and sudoku designs. Finally, in section 5 we consider the moves between different fractions as integer valued functions defined over the full factorial design. We build a procedure to move between fractions that use Markov basis.

2 Notation and background

2.1 Full factorial design

We adopt the notation used in Pistone and Rogantin (2008) and denote:

- by \mathcal{D}_j a *factor* with n_j levels coded with the n_j -th roots of the unity:

$$\mathcal{D}_j = \{\omega_0, \dots, \omega_{n_j-1}\} \quad \omega_k = \exp\left(i \frac{2\pi}{n_j} k\right) ;$$

- by \mathcal{D} the *full factorial design* with *complex coding*

$$\mathcal{D} = \mathcal{D}_1 \times \cdots \mathcal{D}_j \cdots \times \mathcal{D}_m .$$

- by $\#\mathcal{D}$ the cardinality of \mathcal{D} .
- by L the *full factorial design* with *integer coding*

$$L = \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_j} \cdots \times \mathbb{Z}_{n_m} ,$$

- by α an element of L

$$\alpha = (\alpha_1, \dots, \alpha_m) \quad \alpha_j = 0, \dots, n_j - 1, j = 1, \dots, m .$$

- by $[\alpha - \beta]$ the m -tuple made by the componentwise difference

$$([\alpha_1 - \beta_1]_{n_1}, \dots, [\alpha_j - \beta_j]_{n_j}, \dots, [\alpha_m - \beta_m]_{n_m}) ;$$

the computation of the j -th element is in the ring \mathbb{Z}_{n_j} .

- by X_j the j -th component function, which maps a point to its i -th component:

$$X_j : \quad \mathcal{D} \ni (\zeta_1, \dots, \zeta_m) \longmapsto \zeta_j \in \mathcal{D}_j ;$$

the function X_j is called *simple term* or, by abuse of terminology, *factor*.

- by X^α the *interaction term* $X_1^{\alpha_1} \cdots X_m^{\alpha_m}$, i.e. the function

$$X^\alpha : \quad \mathcal{D} \ni (\zeta_1, \dots, \zeta_m) \mapsto \zeta_1^{\alpha_1} \cdots \zeta_m^{\alpha_m} ;$$

We notice that L is both the full factorial design with integer coding and *the exponent set of all the simple factors and interaction terms* and α is both a treatment combination in the integer coding and a multi-exponent of an interaction term.

The full factorial design in complex coding is identified as the zero-set in \mathbb{C}^m of the system of polynomial equations

$$X_j^{n_j} - 1 = 0 \quad , \quad j = 1, \dots, m . \tag{1}$$

Definition 2.1 (1) A response f on the design \mathcal{D} is a \mathbb{C} -valued polynomial function defined on \mathcal{D} .

(2) The mean value on \mathcal{D} of a response f , denoted by $E_{\mathcal{D}}(f)$, is:

$$E_{\mathcal{D}}(f) = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{D}} f(\zeta) .$$

(3) A response f is centered on \mathcal{D} if $E_{\mathcal{D}}(f) = 0$. Two responses f and g are orthogonal on \mathcal{D} if $E_{\mathcal{D}}(f \bar{g}) = 0$, where \bar{g} is the complex conjugate of g .

It should be noticed that the set of all the responses is a complex Hilbert space with the Hermitian product:

$$f \cdot g = E_{\mathcal{D}}(f \bar{g}) .$$

Moreover

- (1) $X^{\alpha} \overline{X^{\beta}} = X^{[\alpha-\beta]}$;
- (2) $E_{\mathcal{D}}(X^0) = 1$, and $E_{\mathcal{D}}(X^{\alpha}) = 0$ for $\alpha \neq 0$.

The set of functions $\{X^{\alpha}, \alpha \in L\}$ is an orthonormal basis of the *complex responses* on design \mathcal{D} . In fact $\#L = \#\mathcal{D}$ and, from properties (i) and (ii) above, it follows that:

$$E_{\mathcal{D}}(X^{\alpha} \overline{X^{\beta}}) = E_{\mathcal{D}}(X^{[\alpha-\beta]}) = \begin{cases} 1 & \text{if } \alpha = \beta \\ 0 & \text{if } \alpha \neq \beta \end{cases}$$

In particular, each response f can be represented as a unique \mathbb{C} -linear combination of constant, simple and interaction terms. This representation is obtained by repeated applications of the re-writing rules derived from Equations (1). Such a polynomial is called the *normal form* of f on \mathcal{D} . In this paper we intend that all the computation are made using the normal form.

Example 2.1 Consider the 2^3 full factorial design. All the monomial responses on \mathcal{D} are

$$1, X_1, X_2, X_3, X_1X_2, X_1X_3, X_2X_3, X_1X_2X_3$$

or, equivalently,

$$X^{(0,0,0)}, X^{(1,0,0)}, X^{(0,1,0)}, X^{(0,0,1)}, X^{(1,1,0)}, X^{(1,0,1)}, X^{(0,1,1)}, X^{(1,1,1)}$$

and L is

$$L = \{(0, 0, 0), (1, 0, 0), (0, 1, 0), (0, 0, 1), (1, 1, 0), (1, 0, 1), (0, 1, 1), (1, 1, 1)\} .$$

2.2 Fractions of a full factorial design

A fraction \mathcal{F} is a multiset (\mathcal{F}_*, f_*) whose underlying set of elements \mathcal{F}_* is contained in \mathcal{D} and f_* is the multiplicity function $f_* : \mathcal{F}_* \rightarrow \mathbb{N}$ that for each element in \mathcal{F}_* gives the number of times it belongs to the multiset \mathcal{F} .

All fractions can be obtained by adding polynomial equations, called *generating equations* to the design equations 1, in order to restrict the number of solutions.

Definition 2.2 *If f is a response on \mathcal{D} then its mean value on \mathcal{F} , denoted by $E_{\mathcal{F}}(f)$, is*

$$E_{\mathcal{F}}(f) = \frac{1}{\#\mathcal{F}} \sum_{\zeta \in \mathcal{F}} f(\zeta)$$

where $\#\mathcal{F}$ is the total number of treatment combinations of the fraction.

A response f is centered if $E_{\mathcal{F}}(f) = 0$. Two responses f and g are orthogonal on \mathcal{F} if $E_{\mathcal{F}}(f \bar{g}) = 0$.

With the complex coding the vector orthogonality of two interaction terms X^α and X^β as defined before (with respect to a given Hermitian product) corresponds to the combinatorial orthogonality (all the level combinations appear equally often in $X^\alpha X^\beta$).

We consider the general case in which fractions can contain points that are replicated.

Definition 2.3 *The counting function R of a fraction \mathcal{F} is a response defined on \mathcal{D} so that for each $\zeta \in \mathcal{D}$, $R(\zeta)$ equals the number of appearances of ζ in the fraction. A 0–1 valued counting function is called indicator function of a single replicate fraction \mathcal{F} . We denote by c_α the coefficients of the representation of R on \mathcal{D} using the monomial basis $\{X^\alpha, \alpha \in L\}$:*

$$R(\zeta) = \sum_{\alpha \in L} c_\alpha X^\alpha(\zeta) \quad \zeta \in \mathcal{D} \quad c_\alpha \in \mathbb{C} .$$

As the counting function is real valued, we have $\overline{c_\alpha} = c_{[-\alpha]}$. We will write c_0 in place of $c_{0,\dots,0}$.

Remark 2.1 *The counting function R coincides with multiplicity function f_* .*

Proposition 2.1 *Let \mathcal{F} be a fraction of a full factorial design \mathcal{D} and $R = \sum_{\alpha \in L} c_\alpha X^\alpha$ be its counting function.*

(1) The coefficients c_α are:

$$c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{F}} \overline{X^\alpha(\zeta)} ;$$

in particular, c_0 is the ratio between the number of points of the fraction and that of the design.

(2) In a fraction without replications, the coefficients c_α are related according to:

$$c_\alpha = \sum_{\beta \in L} c_\beta c_{[\alpha-\beta]} .$$

(3) The term X^α is centered on \mathcal{F} , i.e. $\mathbb{E}_{\mathcal{F}}(X^\alpha) = 0$, if, and only if,

$$c_\alpha = c_{[-\alpha]} = 0 .$$

(4) The terms X^α and X^β are orthogonal on \mathcal{F} , i.e. $\mathbb{E}_{\mathcal{F}}(X^\alpha \overline{X^\beta}) = 0$, if, and only if,

$$c_{[\alpha-\beta]} = 0 .$$

Example 2.2 We consider the fraction $\mathcal{F} = \{(-1, -1, 1), (-1, 1, -1)\}$ of the 2^3 full factorial design of Example 2.1. All the monomial responses on \mathcal{F} and their values on the points are

| ζ | 1 | X_1 | X_2 | X_3 | $X_1 X_2$ | $X_1 X_3$ | $X_2 X_3$ | $X_1 X_2 X_3$ |
|---------------|---|-------|-------|-------|-----------|-----------|-----------|---------------|
| $(-1, -1, 1)$ | 1 | -1 | -1 | 1 | 1 | -1 | -1 | 1 |
| $(-1, 1, -1)$ | 1 | -1 | 1 | -1 | -1 | 1 | -1 | 1 |

Using Item 1 of Proposition 2.1, it is easy to compute the coefficients c_α : $c_{(0,1,0)} = c_{(0,0,1)} = c_{(1,1,0)} = c_{(1,0,1)} = 0$; $c_{(0,0,0)} = c_{(1,1,1)} = \frac{2}{4}$ and $c_{(1,0,0)} = c_{(0,1,1)} = -\frac{2}{4}$. Hence, the indicator function is

$$F = \frac{1}{2} (1 - X_1 - X_2 X_3 + X_1 X_2 X_3) .$$

From the null coefficients we see that X_1 and X_3 are centered and that X_1 is orthogonal to both X_2 and X_3 . \square

2.3 Projectivity and orthogonal arrays

Definition 2.4 A fraction \mathcal{F} factorially projects onto the I -factors, $I \subset \{1, \dots, m\}$, if the projection is a multiple full factorial design, i.e. a full factorial design where each point appears equally often. A fraction \mathcal{F} is a mixed orthogonal array of strength t if it factorially projects onto any I -factors with $\#I = t$.

Strength t means that, for any choice of t columns of the matrix design, all possible combinations of symbols appear equally often.

Proposition 2.2 (Projectivity) (1) *A fraction factorially projects onto the I -factors if, and only if, all the coefficients of the counting function involving only the I -factors are 0.*

- (2) *If there exists a subset J of $\{1, \dots, m\}$ such that the J -factors appear in all the non null elements of the counting function, the fraction factorially projects onto the I -factors, with $I = J^c$.*
- (3) *A fraction is an orthogonal array of strength t if, and only if, all the coefficients of the counting function up to the order t are zero:*

$$c_\alpha = 0 \quad \text{for all } \alpha \text{ of order up to } t, \alpha \neq (0, 0, \dots, 0).$$

Example 2.3 (Orthogonal array) *The fraction of a 2^5 full factorial design*

$$\begin{aligned} \mathcal{F}_O = & \{(-1, -1, -1, -1, -1, 1), (-1, -1, -1, 1, 1, 1), (-1, -1, 1, -1, -1, -1), \\ & (-1, -1, 1, 1, 1, -1), (-1, 1, -1, -1, -1, -1), (-1, 1, -1, 1, 1, -1), (-1, 1, 1, -1, 1, 1), \\ & (-1, 1, 1, 1, -1, 1), (1, -1, -1, -1, 1, 1), (1, -1, -1, 1, -1, 1), (1, -1, 1, -1, 1, -1), \\ & (1, -1, 1, 1, -1, -1), (1, 1, -1, -1, 1, -1), (1, 1, -1, 1, -1, -1), (1, 1, 1, -1, -1, 1), \\ & (1, 1, 1, 1, 1, 1)\} \end{aligned}$$

is an orthogonal array of strength 2; in fact, its indicator function

$$\begin{aligned} F = & \frac{1}{4} + \frac{1}{4}X_2X_3X_6 - \frac{1}{8}X_1X_4X_5 + \frac{1}{8}X_1X_4X_5X_6 + \frac{1}{8}X_1X_3X_4X_5 \\ & + \frac{1}{8}X_1X_2X_4X_5 + \frac{1}{8}X_1X_3X_4X_5X_6 + \frac{1}{8}X_1X_2X_4X_5X_6 \\ & + \frac{1}{8}X_1X_2X_3X_4X_5 - \frac{1}{8}X_1X_2X_3X_4X_5X_6 \end{aligned}$$

contains only terms of order greater than 2, together with the constant term.

□

3 Counting functions and strata

From Proposition 2.1 and Proposition 2.2 we have that the problem of finding fractional factorial designs that satisfy a set of conditions in terms of orthogonality between factors can be written as a polynomial system in which the indeterminates are the complex coefficients c_α of the counting polynomial fraction.

Example 3.1 Let's consider 3 factors, each one with two levels. The indicator functions $F = \sum_{\alpha} c_{\alpha} X^{\alpha}$ such that the terms X_1, X_2, X_3 are centered on \mathcal{F} and the terms X_i, X_j $i, j = 1, 2, 3, i \neq j$ are orthogonal on \mathcal{F} , where $\mathcal{F} = \{\zeta \in \mathcal{D} : F(\zeta) = 1\}$, are those for which the following conditions on the coefficients of F holds

$$\begin{cases} c_0 = c_0^2 + c_{123}^2 \\ c_{123} = 2c_0 c_{123} \end{cases}$$

Apart from the trivial $F = 0$, i.e. $\mathcal{F} = \emptyset$ and $F = 1$, i.e. $\mathcal{F} = \mathcal{D}$ we find $F = \frac{1}{2}(1 + X_1 X_2 X_3)$ and $F = \frac{1}{2}(1 - X_1 X_2 X_3)$

Let's now introduce a different way to describe the full factorial design \mathcal{D} and all its subsets. Let's consider the indicator functions 1_{ζ} of all the single points of \mathcal{D}

$$1_{\zeta} : \quad \mathcal{D} \ni (\zeta_1, \dots, \zeta_m) \mapsto \begin{cases} 1 & \zeta = (\zeta_1, \dots, \zeta_m) \\ 0 & \zeta \neq (\zeta_1, \dots, \zeta_m) \end{cases}$$

It follows that the counting function R of a fraction \mathcal{F} can be written as

$$\sum_{\zeta \in \mathcal{D}} y_{\zeta} 1_{\zeta}$$

with $y_{\zeta} \equiv R(\zeta) \in \{0, 1, \dots, n, \dots\}$. The particular case in which R is an indicator function corresponds to $y_{\zeta} \in \{0, 1\}$.

The coefficients y_{ζ} are related to the coefficients c_{α} as in the following Proposition 3.1

Proposition 3.1 Let \mathcal{F} be a fraction of \mathcal{D} . Its counting fraction R can be expressed both as $R = \sum_{\alpha} c_{\alpha} X^{\alpha}$ and $R = \sum_{\zeta \in \mathcal{D}} y_{\zeta} 1_{\zeta}$. The relation between the coefficients c_{α} and y_{ζ} is

$$c_{\alpha} = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{D}} y_{\zeta} \overline{X^{\alpha}(\zeta)}$$

Proof. From Proposition 2.1 we have

$$\begin{aligned} c_{\alpha} &= \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{F}} \overline{X^{\alpha}(\zeta)} = \\ &= \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{D}} y_{\zeta} \overline{X^{\alpha}(\zeta)} \end{aligned}$$

□

3.1 Strata

As described in Section 2, we consider m factors, $\mathcal{D}_1, \dots, \mathcal{D}_m$ where $\mathcal{D}_j \equiv \Omega_{n_j} = \{\omega_0, \dots, \omega_{n_j-1}\}$, for $j = 1, \dots, m$. From Pistone and Rogantin (2008), we recall two basic properties which hold true for the full design \mathcal{D}

Proposition 3.2 *Let X_j the simple term with level set $\Omega_{n_j} = \{\omega_0, \dots, \omega_{n_j-1}\}$. Let's consider the term X_j^r and let's define*

$$s_j = \begin{cases} 1 & r = 0 \\ n_j/\gcd(r, n_j) & r > 0 \end{cases}$$

Over \mathcal{D} , the term X_j^r takes all the values of Ω_{s_j} equally often.

Proposition 3.3 *Let $X^\alpha = X_1^{\alpha_1} \cdots X_m^{\alpha_m}$ an interaction. $X_i^{\alpha_i}$ takes values in Ω_{s_i} where s_i is determined according to the previous Proposition 3.2. Let's define $s = \text{lcm}(s_1, \dots, s_m)$. Over \mathcal{D} , the term X^α takes all the values of Ω_s equally often.*

Let's now define the strata that are associated to simple and interaction terms.

Definition 3.1 *Given a term $X^\alpha, \alpha \in L = \mathbb{Z}_{n_1} \times \dots \times \mathbb{Z}_{n_m}$ the full design \mathcal{D} is partitioned into the the following strata*

$$D_h^\alpha = \left\{ \zeta \in \mathcal{D} : \overline{X^\alpha(\zeta)} = \omega_h \right\}$$

where $\omega_h \in \Omega_s$ and s is determined according to the previous Propositions 3.2 and 3.3.

Remark 3.1 *We define strata using the conjugate $\overline{X^\alpha}$ of the term in place of the term X^α itself because it will simplify the notations.*

Remark 3.2 *Each stratum is a regular fraction whose defining equation is $X^\alpha(\zeta) = \omega_{-h}$, Pistone and Rogantin (2008).*

We use $n_{\alpha,h}$ to denote the number of points of the fraction \mathcal{F} that are in the stratum D_h^α , with $h = 0, \dots, s - 1$,

$$n_{\alpha,h} = \sum_{\zeta \in D_h^\alpha} y_\zeta$$

The following Proposition 3.4 links the coefficients c_α with $n_{\alpha,h}$.

Proposition 3.4 *Let \mathcal{F} be a fraction of \mathcal{D} with counting fraction $R = \sum_{\alpha \in L} c_\alpha X^\alpha$.*

Each $c_\alpha, \alpha \in L$, depends on $n_{\alpha,h}, h = 0, \dots, s-1$, as

$$c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{h=0}^{s-1} n_{\alpha,h} \omega_h$$

where s is determined by X^α (see Proposition 3.3). Viceversa, each $n_{\alpha,h}, h = 0, \dots, s-1$, depends on $c_{[-k\alpha]}, k = 0, \dots, s-1$ as

$$n_{\alpha,h} = \frac{\#\mathcal{D}}{s} \sum_{k=0}^{s-1} c_{[-k\alpha]} \omega_{[hk]}$$

Proof. Using Proposition 3.1, it follows that we can write the coefficients c_α in the following way

$$c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{D}} y_\zeta \overline{X^\alpha(\zeta)} = \frac{1}{\#\mathcal{D}} \sum_{h=0}^{s-1} \omega_h \sum_{\zeta \in D_h^\alpha} y_\zeta = \frac{1}{\#\mathcal{D}} \sum_{h=0}^{s-1} n_{\alpha,h} \omega_h$$

For the viceversa, we observe the indicator function of strata can be obtained as follows. We define

$$\tilde{F}_0^s(\zeta) = \sum_{k=0}^{s-1} \zeta^k = \begin{cases} \frac{1-\zeta^s}{1-\zeta} & \text{if } \zeta \neq 1 \\ s & \text{if } \zeta = 1 \end{cases}$$

We have $\tilde{F}_0^s(\omega_k) = 0$ for all $\omega_k \in \Omega_s, k \neq 0$. It follows that

$$F_{\alpha,0}(\zeta) = \frac{1}{s} \tilde{F}_0^s(\zeta^\alpha) = \frac{1}{s} (1 + \zeta^\alpha + \dots + \zeta^{(s-1)\alpha})$$

is the indicator function associated to D_0^α .

The indicator of $D_h^\alpha = \{\zeta \in \mathcal{D} : \overline{X^\alpha(\zeta)} = \omega_h\} = \{\zeta \in \mathcal{D} : X^\alpha(\zeta) = \omega_{[-h]}\}$ will be

$$F_{\alpha,h}(\zeta) = F_0^s(\omega_h \zeta^\alpha) = \frac{1}{s} (1 + \omega_h \zeta^\alpha + \dots + \omega_{[(s-1)h]} \zeta^{(s-1)\alpha})$$

We get

$$\begin{aligned} n_{\alpha,h} &= \sum_{\zeta \in D_h^\alpha} R(\zeta) = \sum_{\zeta \in \mathcal{D}} F_{\alpha,h}(\zeta) R(\zeta) = \\ &= \sum_{\zeta \in \mathcal{D}} \left(\frac{1}{s} \sum_{k=0}^{s-1} \omega_{[kh]} X^{k\alpha}(\zeta) \right) \left(\sum_{\beta} c_\beta X^\beta(\zeta) \right) = \\ &= \frac{\#\mathcal{D}}{s} \sum_{k,\beta: [k\alpha+\beta]=0} \omega_{[kh]} c_\beta = \frac{\#\mathcal{D}}{s} \sum_{k=0}^{s-1} \omega_{[kh]} c_{[-k\alpha]} \end{aligned}$$

□

Remark 3.3 From Proposition 3.4 we get

$$n_{0,h} = 0, \quad h = 1, \dots, s - 1$$

$$n_{\alpha,0} = \frac{\#\mathcal{D}}{s} \sum_{k=0}^{s-1} c_{[-k\alpha]}$$

and in particular $n_{0,0} = \#\mathcal{F}$.

We now use a part of Proposition 3 of Pistone and Rogantin (2008) to get conditions on $n_{\alpha,h}$ that makes X^α centered on the fraction \mathcal{F} .

Proposition 3.5 Let X^α be a term with level set Ω_s on full design \mathcal{D} . Let $P(\zeta)$ the complex polynomial associated to the sequence $(n_{\alpha,h})_{h=0,\dots,s-1}$ so that

$$P(\zeta) = \sum_{h=0}^{s-1} n_{\alpha,h} \zeta^h$$

and let's denote by Φ_s the cyclotomic polynomial of the s -roots of the unity.

- (1) Let s be prime. The term X^α is centered on the fraction \mathcal{F} if, and only if, its s levels appear equally often:

$$n_{\alpha,0} = n_{\alpha,1} = \dots = n_{\alpha,s-1} = \lambda_\alpha$$

- (2) Let $s = p_1^{h_1} \dots p_d^{h_d}$ with p_i prime, for $i = 1, \dots, d$. The term X^α is centered on the fraction \mathcal{F} if, and only if, the remainder

$$H(\zeta) = P(\zeta) \bmod \Phi_s(\zeta)$$

whose coefficients are integer linear combinations of $n_{\alpha,h}$, $h = 0, \dots, s-1$, is identically zero.

Proof. See Proposition 3 of Pistone and Rogantin (2008). \square

Remark 3.4 Being D_h^α a partition of \mathcal{D} , if s is prime we get $\lambda_\alpha = \frac{\#\mathcal{F}}{s}$.

If we remind that $n_{\alpha,h}$ are related to the values of the counting function R of a fraction \mathcal{F} by the following relation

$$n_{\alpha,h} = \sum_{\zeta \in D_h^\alpha} y_\zeta,$$

this Proposition 3.5 allows to express the condition X^α is centered on \mathcal{F} as integer linear combinations of the values $R(\zeta)$ of the counting function over the full design \mathcal{D} . In the Section 4, we will show the use of this property to generate fractional factorial designs.

We conclude this section limiting to the particular case where all factors have the same number of levels s and s is prime. We provide some results concerning the coefficients of counting functions, regular fractions, wordlength patterns and margins.

3.2 Coefficients of the polynomial counting function

From Proposition 3.5 we get the following result on the coefficients of a counting function

Proposition 3.6 *Given a counting function $R = \sum_{\alpha} c_{\alpha} X^{\alpha}$, if $c_{\alpha} = 0$ then $c_{[k \cdot \alpha]} = 0$ for all $k = 1, \dots, s - 1$, where $[k \cdot \alpha]$ is $\underbrace{\alpha + \dots + \alpha}_{k \text{ times}}$ in the ring \mathbb{Z}_s^m .*

Proof. Let's consider $c_{k \cdot \alpha}$. From Proposition 3.5, $c_{k \cdot \alpha}$ is equal to zero if, and only if,

$$\sum_{\zeta \in D_0^{k \cdot \alpha}} y_{\zeta} = \sum_{\zeta \in D_1^{k \cdot \alpha}} y_{\zeta} = \dots = \sum_{\zeta \in D_{s-1}^{k \cdot \alpha}} y_{\zeta}$$

We observe that

$$\begin{aligned} D_h^{k \cdot \alpha} &= \left\{ \zeta \in \mathcal{D} : \overline{X^{k \cdot \alpha}(\zeta)} = \omega_h \right\} = \\ &= \left\{ \zeta \in \mathcal{D} : \overline{X^{\alpha}(\zeta)}^k = \omega_h \right\} = \left\{ \zeta \in \mathcal{D} : \overline{X^{\alpha}(\zeta)} = \omega_{[kh]} \right\} = D_{[kh]}^{\alpha} \end{aligned}$$

where $[kh]$ is $\underbrace{h + \dots + h}_{k \text{ times}}$ in the ring \mathbb{Z}_s .

It follows that X^{α} and $X^{k \cdot \alpha}$ partition \mathcal{D} in the same strata and therefore we get the proof. \square

3.3 Regular designs

Let's consider a fraction \mathcal{F} without replicates and with indicator function $F = \sum_{\alpha} c_{\alpha} X^{\alpha}$. Proposition 5 in (Pistone and Rogantin (2008)) states that a fraction \mathcal{F} is regular if, and only if, its indicator function F has the form

$$F = \frac{1}{l} \sum_{\alpha \in \mathcal{L}} \overline{e(\alpha)} X^{\alpha}$$

where $\mathcal{L} \subseteq L$, \mathcal{L} is a subgroup of L and $e : \mathcal{L} \rightarrow \{\omega_0, \dots, \omega_{s-1}\}$ is a given mapping.

If we use Proposition 3.5 we immediately get a characterisation of regular fractions based on the frequencies $n_{\alpha,h}$.

Proposition 3.7 *Given a single replicate fraction \mathcal{F} with indicator function $F = \sum_{\alpha} c_{\alpha} X^{\alpha}$ the following statements are equivalent:*

- (i) \mathcal{F} is regular
- (ii) for $n_{\alpha,h}$ there are only two possibilities
 - (a) if $c_{\alpha} = 0$ then $n_{\alpha,h} = \frac{\#\mathcal{F}}{s}$, $h = 0, \dots, s-1$,
 - (b) if $c_{\alpha} \neq 0$ then $\exists h_* \in \{0, \dots, s-1\}$ such that

$$n_{\alpha,h} = \begin{cases} \frac{\#\mathcal{D}}{l} & \text{if } h = h_* \\ 0 & \text{otherwise} \end{cases}$$

Proof. Using Proposition 3.4 we get

$$c_{\alpha} = \frac{1}{\#\mathcal{D}} \sum_{h=0}^{s-1} n_{\alpha,h} \omega_h$$

Proposition 5 in Pistone and Rogantin (2008) gives the following conditions on the coefficients of the indicator function F of a regular fraction \mathcal{F} :

$$c_{\alpha} = \begin{cases} \frac{\overline{e(\alpha)}}{l}, & \alpha \in \mathcal{L} \subseteq L \\ 0 & \text{otherwise} \end{cases}$$

where $e : \mathcal{L} \rightarrow \{\omega_0, \dots, \omega_{s-1}\}$, $l = \#\mathcal{L}$ and \mathcal{L} is a subgroup of L .

Let's consider $\alpha \in \mathcal{L}$. We get

$$\frac{1}{\#\mathcal{D}} \sum_{h=0}^{s-1} n_{\alpha,h} \omega_h = \frac{\overline{e(\alpha)}}{l}$$

Let's suppose $e(\alpha) = \omega_{h_*}$. We obtain

$$\frac{1}{\#\mathcal{D}} \sum_{h=0, h \neq h_*}^{s-1} n_{\alpha,h} \omega_h + \left(\frac{1}{\#\mathcal{D}} n_{\alpha,h_*} - \frac{1}{l} \right) \omega_{h_*} = 0 \quad (2)$$

To simplify the notation we let $a_h = \frac{1}{\#\mathcal{D}} n_{\alpha,h}$, $h = 0, \dots, s-1$, $h \neq h_*$ and $a_{h_*} = \frac{1}{\#\mathcal{D}} n_{\alpha,h_*} - \frac{1}{l}$. Therefore, from the proof of item (1) of Proposition 3.5, for the relation 2 to be valid, it should be

$$a_0 = a_1 = \dots = a_{s-1}$$

Being $\sum_{h=0}^{s-1} n_{\alpha,h} = \#\mathcal{F}$ it follows

$$\sum_{h=0}^{s-1} n_{\alpha,h} = \sum_{h=0, h \neq h_*}^{s-1} (\#\mathcal{D}) a_h + (\#\mathcal{D}) (a_{h_*} + \frac{1}{l}) = (\#\mathcal{D}) \sum_{h=0}^{s-1} a_h + \frac{(\#\mathcal{D})}{l} = \#\mathcal{F}$$

and so

$$a_h = \frac{1}{s(\#\mathcal{D})} (\#\mathcal{F} - \frac{(\#\mathcal{D})}{l})$$

We finally get

$$n_{\alpha,h} = \begin{cases} \frac{1}{s} (\#\mathcal{F} - \frac{(\#\mathcal{D})}{l}) + \frac{(\#\mathcal{D})}{l} & \text{if } h = h_* \\ \frac{1}{s} (\#\mathcal{F} - \frac{(\#\mathcal{D})}{l}) & \text{otherwise} \end{cases}$$

Being \mathcal{L} a subgroup of L it follows that $0 \in \mathcal{L}$ and so $c_0 = 1/l$. We also know that $c_0 = \frac{\#\mathcal{F}}{\#\mathcal{D}}$ and therefore

$$\#\mathcal{F} = \frac{\#\mathcal{D}}{l}$$

For the null coefficients of F , $\{c_\alpha : \alpha \in L - \mathcal{L}\}$, it is enough to use Proposition ?? to conclude the proof. \square

3.4 Wordlength Pattern

Aberration is often used as a criterion to compare fractional factorial designs. The generalized minimum aberration, proposed by Xu and Wu (2001), is based on the generalised wordlength pattern, see also Beder and Willenbring (2009). It can be shown that the generalized wordlengths can be written in terms of the squares of the modules of the coefficients c_α , obtaining

$$A_j = \left(\frac{\#\mathcal{D}}{\#\mathcal{F}} \right)^2 \sum_{wt(\alpha)=j} |c_\alpha|^2 = \frac{1}{c_0^2} \sum_{wt(\alpha)=j} |c_\alpha|^2 \quad \text{for } j = 1, \dots, m$$

where $wt(\alpha)$ is the Hamming weight of α , i.e. the number of nonzero components of α . We now express the square of the module of the coefficient c_α in terms of $n_{\alpha,h}$.

Proposition 3.8

$$|c_\alpha|^2 = \frac{1}{(\#\mathcal{D})^2} \sum_{h=0}^{s-1} (n_{\alpha,h}^2 - n_{\alpha,h} n_{[\alpha,h-\gamma]}) \quad \text{for } \gamma \in \{1, \dots, s-1\}$$

Proof. From Proposition 3.4 we get

$$c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{h=0}^{s-1} n_{\alpha,h} \omega_h$$

It follows

$$\begin{aligned}
|c_\alpha|^2 &= c_\alpha \overline{c_\alpha} = \\
&= \frac{1}{(\#\mathcal{D})^2} \left(\sum_{h=0}^{s-1} n_{\alpha,h} \omega_h \right) \left(\sum_{k=0}^{s-1} n_{\alpha,k} \overline{\omega_k} \right) = \\
&= \frac{1}{(\#\mathcal{D})^2} \left(\sum_{h=0}^{s-1} n_{\alpha,h} \omega_h \right) \left(\sum_{k=0}^{s-1} n_{\alpha,k} \omega_{[s-k]} \right) = \\
&= \frac{1}{(\#\mathcal{D})^2} \sum_{\gamma=0}^{s-1} \sum_{p=0}^{s-1} n_{\alpha,p} n_{[\alpha,p-\gamma]} \omega_\gamma
\end{aligned}$$

$|c_\alpha|^2$ must be a real number. Being $\omega_0 = 1$ it follows

$$\left(\frac{1}{(\#\mathcal{D})^2} \sum_{p=0}^{s-1} n_{\alpha,p}^2 - |c_\alpha|^2 \right) \omega_0 + \frac{1}{(\#\mathcal{D})^2} \sum_{\gamma=1}^{s-1} \sum_{p=0}^{s-1} n_{\alpha,p} n_{[\alpha,p-\gamma]} \omega_\gamma = 0 \quad (3)$$

To simplify the notation we let $a_0 = (\frac{1}{(\#\mathcal{D})^2} \sum_{p=0}^{s-1} n_{\alpha,p}^2 - |c_\alpha|^2)$ and $a_\gamma = \frac{1}{(\#\mathcal{D})^2} \sum_{p=0}^{s-1} n_{\alpha,p} n_{[\alpha,p-\gamma]}$, $\gamma = 1, \dots, s-1$. Therefore, by Lemma ??, for the relation 3 to be valid, it should be

$$a_0 = a_1 = \dots = a_{s-1}$$

Using one of the equalities, $a_0 = a_h$ $h = 1, \dots, s-1$, it follows

$$|c_\alpha|^2 = \frac{1}{(\#\mathcal{D})^2} \sum_{p=0}^{s-1} (n_{\alpha,p}^2 - n_{\alpha,p} n_{[\alpha,p-h]}) \quad (3)$$

□

Remark 3.5 Proposition 3.8 provides a useful tool to compute the modules of the coefficients c_α . Indeed it is enough to choose $\gamma = 1$ and compute $|c_\alpha|^2$ as $\frac{1}{(\#\mathcal{D})^2} \sum_{h=0}^{s-1} (n_{\alpha,h}^2 - n_{\alpha,h} n_{[\alpha,h-1]})$;

Remark 3.6 We make explicit these relations for 2 and 3 level fraction.

If $s = 2$ then

$$|c_\alpha|^2 = \frac{1}{(\#\mathcal{D})^2} (n_{\alpha,0} - n_{\alpha,1})^2$$

If $s = 3$ then, choosing $\gamma = 1$,

$$|c_\alpha|^2 = \frac{1}{(\#\mathcal{D})^2} (n_{\alpha,0}^2 + n_{\alpha,1}^2 + n_{\alpha,2}^2 - n_{\alpha,0} n_{\alpha,2} - n_{\alpha,1} n_{\alpha,0} - n_{\alpha,2} n_{\alpha,1})$$

Remark 3.7 We observe that, denoting by \bar{n}_α the mean of the values of $n_{\alpha,h}$,

$\bar{n}_\alpha = \frac{1}{s} \sum_{h=0}^{s-1} n_{\alpha,h}$, we get

$$\sum_{h=0}^{s-1} (n_{\alpha,h} - \bar{n}_\alpha)^2 = \sum_{h=0}^{s-1} n_{\alpha,h}^2 - s\bar{n}_\alpha^2$$

We have

$$\begin{aligned} \bar{n}_\alpha^2 &= \frac{1}{s^2} \sum_{h,k=0}^{s-1} n_{\alpha,h} n_{\alpha,k} = \\ &= \frac{1}{s^2} \left(\sum_{h=0}^{s-1} n_{\alpha,h}^2 + 2 \sum_{h=0}^{s-1} n_{\alpha,h} n_{\alpha,[h-1]} + \dots + 2 \sum_{h=0}^{s-1} n_{\alpha,h} n_{\alpha,[h-s_*]} \right) \end{aligned}$$

where $s_* = \frac{s-1}{2}$. Proposition 3.8 states that all the quantities $\sum_{h=0}^{s-1} n_{\alpha,h} n_{\alpha,[h-\gamma]}$ are equal and so, choosing, without loss of generality, $\gamma = 1$, we get

$$\bar{n}_\alpha^2 = \frac{1}{s^2} \left(\sum_{h=0}^{s-1} n_{\alpha,h}^2 + 2s_* \sum_{h=0}^{s-1} n_{\alpha,h} n_{\alpha,[h-1]} \right) = \frac{1}{s^2} \left(\sum_{h=0}^{s-1} n_{\alpha,h}^2 + (s-1) \sum_{h=0}^{s-1} n_{\alpha,h} n_{\alpha,[h-1]} \right)$$

and therefore

$$\begin{aligned} \sum_{h=0}^{s-1} (n_{\alpha,h} - \bar{n}_\alpha)^2 &= \sum_{h=0}^{s-1} n_{\alpha,h}^2 - s\bar{n}_\alpha^2 = \\ &= \frac{s-1}{s} \left(\sum_{h=0}^{s-1} n_{\alpha,h}^2 - \sum_{h=0}^{s-1} n_{\alpha,h} n_{\alpha,[h-1]} \right) = \\ &= \frac{s-1}{s} (\#\mathcal{D})^2 |c_\alpha|^2 \end{aligned}$$

It follows that, if we denote by σ_α^2 the variance of $n_{\alpha,h}$, $\sigma_\alpha^2 = \frac{1}{s} \sum_{h=0}^{s-1} (n_{\alpha,h} - \bar{n}_\alpha)^2$ we get

$$|c_\alpha|^2 = \left(\frac{s^2}{(s-1)(\#\mathcal{D})^2} \right) \sigma_\alpha^2$$

and so the square of the module of c_α represents, apart from a multiplicative constant, the variance of the frequencies $n_{\alpha,h}$.

3.5 Margins

We now examine the relationship between the margins and the coefficients of the counting functions. We refer to (Pistone and Rogantin (2008)) and we report here a part of it.

For each point $\zeta \in \mathcal{D}$ we consider the decomposition $\zeta = (\zeta_I, \zeta_J)$ where $I \subseteq \{1, \dots, m\}$ and $J = \{1, \dots, m\} - I \equiv I^c$ is its complement. We denote by $R_I(\zeta_I)$ the number of points in \mathcal{F} whose projection on the I factors is ζ_I .

In particular if $I = \{1, \dots, m\}$ we have $R_I = R$ and if $I = \emptyset$ we have $R_I = \#\mathcal{F}$.

We denote by L_I the subset of the exponents restricted to the I factors and by α_I an element of L_I :

$$L_I = \{\alpha_I = (\alpha_1, \dots, \alpha_m), \alpha_j = 0 \text{ if } j \in J\}$$

Then for each $\alpha \in L$ and $\zeta \in \mathcal{D}$ we have $\alpha = \alpha_I + \alpha_J$ and $X^\alpha(\zeta) = X_I^\alpha(\zeta_I)X_J^\alpha(\zeta_J)$. Finally we denote by \mathcal{D}_I and \mathcal{D}_J the full factorial over the I factors and J factors, respectively ($\mathcal{D} = \mathcal{D}_I \times \mathcal{D}_J$).

We have the following proposition (see item 1 and 2 of Proposition 4 of Pistone and Rogantin (2008))

Proposition 3.9 *Given a fraction \mathcal{F} of \mathcal{D}*

(1) *the number of replicates of the points of \mathcal{F} projected on the I factors is:*

$$R_I(\zeta_I) = \#\mathcal{D}_J \sum_{\alpha_I} c_{\alpha_I} X^{\alpha_I}(\zeta_I)$$

(2) *\mathcal{F} fully projects on the I factors if, and only if,*

$$R_I(\zeta_I) = \#\mathcal{D}_J \cdot c_0 = \#\mathcal{D}_J \frac{\#\mathcal{F}}{\#\mathcal{D}} = \frac{\#\mathcal{F}}{\#\mathcal{D}_I}$$

We will refer to R_I as k -margin, where $k = \#I$. The number of k -margins is $\binom{m}{k}$ and each k -margin can be computed over s^k points $\zeta_I \in \mathcal{D}_I$. It follows that there are $(1+s)^m$ marginal values in total.

Using item 1 of Proposition 3.9 and reminding that we work with a prime number of level s we have

$$R_I(\zeta_I) = s^{m-k} \sum_{\alpha_I} c_{\alpha_I} \zeta_I^{\alpha_I}$$

or, by the definition of R_I as the restriction of R over the I factors,

$$\sum_{\zeta_J \in \mathcal{D}_J} R(\zeta_I, \zeta_J) \equiv \sum_{\zeta_J \in \mathcal{D}_J} y_{\zeta_I, \zeta_J} = s^{m-k} \sum_{\alpha_I} c_{\alpha_I} \zeta_I^{\alpha_I}$$

We point out the following relationship between margins.

Proposition 3.10 *If $A \subseteq B \subseteq \{1, \dots, m\}$ and $R_B(\zeta_B) = s^{m-k_B} c_0$ then $R_A(\zeta_A) = s^{m-k_A} c_0$ where $\#B = k_B$ and $\#A = k_A$*

Proof. Let's put $A_1 = B - A$. We have

$$R_A(\zeta_A) = \sum_{\zeta_{A_1} \in A_1} R_{A \cup A_1}(\zeta_A, \zeta_{A_1}) = \sum_{\zeta_{A_1} \in A_1} R_B(\zeta_A, \zeta_{A_1}) = s^{k_B - k_A} s^{m - k_B} c_0 = s^{m - k_A} c_0$$

□

We finally observe that, as we already pointed out, given $\mathcal{C} \subseteq L$ a set of conditions $c_\alpha = 0, \alpha \in \mathcal{C}$ translates in a set of conditions $\sum_{\zeta \in D_h^\alpha} y_\zeta = \lambda, h = 0, \dots, s-1, \alpha \in \mathcal{C}$ where λ does not depend by α (and by h). In general, with respect to margins, the situation is different. For example let's suppose to have a \mathcal{F} that fully projects over the I_1 and the I_2 factors, with $I_1 \cap I_2 = \emptyset$ and $\#I_1 \neq \#I_2$. From Proposition 3.9 we obtain

$$R_{I_1}(\zeta_{I_1}) = \frac{\#\mathcal{D}}{s^{\#I_1}} \text{ and } R_{I_2}(\zeta_{I_2}) = \frac{\#\mathcal{D}}{s^{\#I_2}}$$

4 Generation of fractions

Let use strata to generate fractions that satisfy a given set of constraints on the coefficients of their counting functions. Formally we give the following definition

Definition 4.1 *A counting function $R = \sum_\alpha c_\alpha X^\alpha$ associated to \mathcal{F} is a \mathcal{C} -compatible counting function if its coefficients satisfy to*

$$c_\alpha = 0, \alpha \in \mathcal{C}, \mathcal{C} \subseteq \mathbb{Z}_{n_1} \times \dots \mathbb{Z}_{n_m}$$

We will denote by $OF(n_1 \dots n_m, \mathcal{C})$ the set of all the fractions whose counting functions are \mathcal{C} -compatible.

In the next sections, we will show our methodology on Orthogonal Arrays and Sudoku designs.

4.1 $OA(n, s^m, t)$

Let's consider $OA(n, s^m, t)$, i.e. orthogonal arrays with n rows and m columns where each column has s symbols, s prime and with strength t .

Using Proposition 2.2 we have that the coefficients of the corresponding counting functions must satisfy the conditions $c_\alpha = 0$ for all $\alpha \in \mathcal{C}$ where $\mathcal{C} \subseteq L = \{\alpha : 0 < \|\alpha\| \leq t\}$ where $\|\alpha\|$ is the number of non null elements of α . We have $N_1 = \sum_{k=1}^t \binom{m}{k} (s-1)^k$ coefficients that must be null.

It follows that $OF(s^m, \mathcal{C}) = \bigcup_n OA(n, s^m, t)$.

Now using Proposition 3.5, we can express these conditions using strata. If we consider $\alpha \in \mathcal{C}$ we write the condition $c_\alpha = 0$ as

$$\begin{cases} \sum_{\zeta \in D_0^\alpha} y_\zeta = \lambda \\ \sum_{\zeta \in D_1^\alpha} y_\zeta = \lambda \\ \dots \\ \sum_{\zeta \in D_{s-1}^\alpha} y_\zeta = \lambda \end{cases}$$

To obtain all the conditions it is enough to vary $\alpha \in \mathcal{C}$. We use Proposition 3.6 to limit to the α that give different strata. It is easy to show that we obtain $N_2 = \frac{N_1}{s-1}$ different α , each of them generate s linear equations, for a total of

$$N = sN_2 = s \sum_{k=1}^t \binom{m}{k} (s-1)^{k-1}$$

constraints on the values of the counting function over \mathcal{D} .

We therefore get the following system of linear equations

$$AY = \lambda \underline{1}$$

where A is the $(N \times s^m)$ matrix whose rows contains the values, over \mathcal{D} , of the indicator function of the strata, $1_{D_h^\alpha}$, Y is the s^m column vector whose entries are the values of the counting function over \mathcal{D} , λ will be equal to $\frac{\#\mathcal{F}}{s}$ and $\underline{1}$ is the s^m column vector whose entries are all equal to 1. We can write an equivalent homogeneous system if we consider λ as a new variable. We obtain

$$\tilde{A}\tilde{Y} = 0$$

where

$$\tilde{A} = \left[A \begin{array}{c|c} -1 & \\ \hline -1 & \\ \dots & \\ -1 & \end{array} \right] = [A, -\underline{1}]$$

and

$$\tilde{Y} = \begin{bmatrix} Y \\ \lambda \end{bmatrix} = (Y, \lambda)$$

In an equivalent way, we can also express the conditions $c_\alpha = 0$ for all $\alpha \in \mathcal{C}$

in terms of margins. We obtain

$$R_I(\zeta_I) = s^{m-(\#I)} c_0$$

where $I \subseteq \{1, \dots, m\}$ and $1 \leq \#I \leq t$. If we recall Proposition 3.10, we can limit to the margins R_I where $\#I = t$. We have $s^t \binom{m}{t}$ values of such t margin

$$\sum_{\zeta_J \in \mathcal{D}_J} y_{\zeta_I, \zeta_J} = s^{m-t} c_0$$

In this case, with the same approach that we adopted for strata, we obtain a system of linear equations

$$BY = \rho \underline{1}$$

where $\rho = s^{m-t} c_0$ and its equivalent homogeneous system

$$\tilde{B}\tilde{Y} = 0$$

Now we can find all the generators of $OF(s^m, \mathcal{C}$, that means of Orthogonal Arrays $OA(n, s^m, t)$, by computing the Hilbert Basis corresponding to \tilde{A} (or, equivalently, to \tilde{B}). This approach is the same of Carlini and Pistone (2007) but, in that work, the following conditions were used

$$c_\alpha = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{F}} \overline{X^\alpha(\zeta)} = \frac{1}{\#\mathcal{D}} \sum_{\zeta \in \mathcal{D}} \overline{X^\alpha(\zeta)} y_\zeta = 0$$

The advantage of using strata (or margins) is that we avoid computations with complex numbers ($\overline{X^\alpha(\zeta)}$). We explain this point in a couple of examples. For the computation we use 4ti2 (4ti2 team (2007)).

We use both \tilde{A} (strata) and \tilde{B} (margins) because, even if they are fully equivalent from the point of view of the solutions that they generate, they perform differently from the point of view of the computational speed.

4.1.1 $OA(n, 2^5, 2)$

$OA(n, 2^5, 2)$ were investigated in Carlini and Pistone (2007). We build both the matrix \tilde{A} and \tilde{B} . They have 30 rows and 40 rows, respectively and 33 columns. We find the same 26,142 solutions as in the cited paper.

4.1.2 $OA(n, 3^3, 2)$

We build both the matrix \tilde{A} and \tilde{B} . They have 54 rows and 27 rows, respectively and 28 columns. We find 66 solutions, 12 have 9 points, all different and 54 have 18 points, 17 different.

Finally we point out that 4ti2 allows to specify upper bounds for variables. For example, if we use \tilde{B} and we are interested in single replicate orthogonal arrays, we can set 1 as the upper bound for $y_\zeta, \zeta \in \mathcal{D}$. The upper bound for the variable ρ can be set to $s^{m-t} \equiv 3^{3-2}$ that corresponds to $c_0 = 1$, i.e. to the full design \mathcal{D} .

4.2 $OA(n, n_1 \dots n_m, t)$

Let's now consider the general case in which we do not put restrictions on the number of levels.

4.2.1 $OA(n, 4^2, 1)$

In this case the number of levels is a power of a prime, 2^2 . Using Proposition 2.2 we have that the coefficients of the corresponding counting functions must satisfy the conditions $c_\alpha = 0$ for all $\alpha \in \mathcal{C}$ where $\mathcal{C} \subseteq L = \{\alpha : \|\alpha\| = 1\}$.

Let's consider $c_{1,0}$. From Proposition 3.2 we have that X_1 takes the values in Ω_s where $s = 4$. From Proposition 3.5, X_1 will be centered on \mathcal{F} if, and only if, the remainder

$$H(\zeta) = P(\zeta) \bmod \Phi_4(\zeta)$$

is identically zero. We have $\Phi_4(\zeta) = 1 + \zeta^2$ (see Lang (1965)) and so we can compute the remainder

$$H(\zeta) = n_{(1,0),0} - n_{(1,0),2} + (n_{(1,0),1} - n_{(1,0),3})\zeta$$

The condition $H(\zeta)$ identically zero translates into

$$\begin{cases} n_{(1,0),0} - n_{(1,0),2} = 0 \\ n_{(1,0),1} - n_{(1,0),3} = 0 \end{cases}$$

Let's now consider $c_{2,0}$. From Proposition 3.2 we have that X_1^2 takes the values in Ω_s where $s = 2$. From Proposition 3.5, X_1^2 will be centered on \mathcal{F} if, and only if, the remainder

$$H(\zeta) = P(\zeta) \bmod \Phi_2(\zeta)$$

is identically zero. We have $\Phi_2(\zeta) = 1 + \zeta$ (see Lang (1965)) and so we can compute the remainder

$$H(\zeta) = n_{(2,0),0} - n_{(2,0),1}$$

If we repeat the same procedure for all the α such that $\|\alpha\| = 1$ and we recall that

$$n_{\alpha,h} = \sum_{\zeta \in D_h^\alpha} y_\zeta$$

orthogonal arrays $OA(n, 4^2, 1)$ become the integer solutions of the following integer linear homogeneous system

$$\left[\begin{array}{cccccccccccccccc} 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{array} \right] \begin{array}{c} y_{00} \\ y_{10} \\ y_{20} \\ y_{30} \\ y_{01} \\ y_{11} \\ y_{21} \\ y_{31} \\ y_{02} \\ y_{12} \\ y_{22} \\ y_{32} \\ y_{03} \\ y_{13} \\ y_{23} \\ y_{33} \end{array}$$

Using 4ti2 we find 24 solutions that correspond to all the Latin Hypercube Designs (LHD).

4.2.2 $OA(n, 6^2, 1)$

As in the previous examples, using Proposition 2.2 we have that the coefficients of the corresponding counting functions must satisfy the conditions $c_\alpha = 0$ for all $\alpha \in \mathcal{C}$ where $\mathcal{C} \subseteq L = \{\alpha : \|\alpha\| = 1\}$.

Let's consider $c_{1,0}$. From Proposition 3.2 we have that X_1 takes the values in Ω_s where $s = 6$. From Proposition 3.5, X_1 will be centered on \mathcal{F} if, and only if, the remainder

$$H(\zeta) = P(\zeta) \bmod \Phi_6(\zeta)$$

is identically zero. We have $\Phi_6(\zeta) = 1 - \zeta + \zeta^2$ (see Lang (1965)) and so we can compute the remainder

$$H(\zeta) = n_{(1,0),0} - n_{(1,0),2} - n_{(1,0),3} + n_{(1,0),6} + (n_{(1,0),1} + n_{(1,0),2} - n_{(1,0),5} - n_{(1,0),6})\zeta$$

If we repeat the same procedure for all the α such that $\|\alpha\| = 1$ and we recall that

$$n_{\alpha,h} = \sum_{\zeta \in D_h^\alpha} y_\zeta$$

orthogonal arrays $OA(n, 6^2, 1)$ become the integer solutions of an integer linear homogeneous system $AR = 0$ where the matrix A is built as in the previous case of $OA(n, 4^2, 1)$. Using 4ti2 we find 620 solutions that correspond to all the Latin Hypercube Designs (LHD).

4.3 Sudoku designs

As shown in Fontana and Rogantin (2008), a sudoku can be described using its indicator function. Here we report a very short synthesis of Section 1.3 of that work.

A $p^2 \times p^2$ with p prime sudoku design can be seen as a fraction \mathcal{F} of the full factorial design \mathcal{D} :

$$\mathcal{D} = R_1 \times R_2 \times C_1 \times C_2 \times S_1 \times S_2$$

where each factor is coded with the p -th roots of the unity. R_1 and R_2 , C_1 and C_2 , S_1 and S_2 , represent the rows, the columns and the symbols of the sudoku grid, respectively.

The following proposition (Proposition 5 of Fontana and Rogantin (2008)) holds.

Proposition 4.1 *Let F be the indicator function of a fraction \mathcal{F} of a design design, $F = \sum_{\alpha \in L} b_\alpha X^\alpha$. The fraction \mathcal{F} corresponds to a sudoku grid if and only if the coefficients b_α satisfy the following conditions:*

- (1) $b_{000000} = 1/p^2$, i.e. the ratio between the number of points of the fraction and the number of points of the full factorial design is $1/p^2$;
- (2) for all $i_j \in \{0, 1, \dots, p-1\}$:
 - (a) $b_{i_1 i_2 i_3 i_4 00} = 0$ for $(i_1, i_2, i_3, i_4) \neq (0, 0, 0, 0)$,
 - (b) $b_{i_1 i_2 00 i_5 i_6} = 0$ for $(i_1, i_2, i_5, i_6) \neq (0, 0, 0, 0)$,
 - (c) $b_{00 i_3 i_4 i_5 i_6} = 0$ for $(i_3, i_4, i_5, i_6) \neq (0, 0, 0, 0)$,
 - (d) $b_{i_1 0 i_3 0 i_5 i_6} = 0$ for $(i_1, i_3, i_5, i_6) \neq (0, 0, 0, 0)$
 i.e. the fraction factorially projects onto the first four factors and onto both symbol factors and row/column/box factors, respectively.

From this Proposition, we define \mathcal{C} as the union of \mathcal{C}_1 , \mathcal{C}_2 , \mathcal{C}_3 and \mathcal{C}_4 , where

$$\begin{aligned}\mathcal{C}_1 &= \{(i_1 i_2 i_3 i_4 00) : (i_1, i_2, i_3, i_4) \neq (0, 0, 0, 0)\} \\ \mathcal{C}_2 &= \{(i_1 i_2 00 i_5 i_6) : (i_1, i_2, i_5, i_6) \neq (0, 0, 0, 0)\} \\ \mathcal{C}_3 &= \{(00 i_3 i_4 i_5 i_6) : (i_3, i_4, i_5, i_6) \neq (0, 0, 0, 0)\} \\ \mathcal{C}_4 &= \{(i_1 0 i_3 0 i_5 i_6) : (i_1, i_3, i_5, i_6) \neq (0, 0, 0, 0)\}\end{aligned}$$

The problem of finding Sudoku becomes equivalent to find \mathcal{C} -compatible counting functions, that are (i) indicator functions and (ii) that satisfy the additional requirement $b_0 = 1/p^2$.

4.3.1 4×4 Sudoku

We use the conditions \mathcal{C} to build both the matrices \tilde{A} and \tilde{B} . \tilde{A} has 78 rows. With respect to \tilde{B} , that corresponds to the margins that must be constant, if we recall Proposition 3.10 we obtain 64 constraints, all corresponding to 4-margins.

To find all sudoku we use 4ti2, specifying the upper bounds for all the 65 variables. The upper bounds for $y_\zeta, \zeta \in \mathcal{D}$ must be equal to 1. If we use \tilde{A} , the upper bound for λ must be set equal to $\frac{\#\mathcal{F}}{s} \equiv \frac{16}{2} = 8$, while if we use \tilde{b} the upper bound for ρ must be set equal to $s^{m-k} b_0 \equiv 2^{2\frac{1}{4}} = 1$.

We find all the 288 different 4×4 sudoku as in Fontana and Rogantin (2008). We point out that to solve the problem using \tilde{A} the total time was 31.59 minutes, while using \tilde{B} the total time was only 58.04 seconds on the same computer.

If we admit counting functions with values in $\{0, 1, 2\}$ and $\#\mathcal{F} \leq 32$ we find 55,992 solutions.

5 Moves

Sometimes, given a set of conditions \mathcal{C} we are interested in picking up a solution more than in finding all the generators. The basic idea is to generate somehow a starting solution and then to randomly walk in the set of all the solutions for a certain number of steps, taking the arrival point as a new but still \mathcal{C} -compatible counting function.

Let's use the previous results on strata to get a suitable set of *moves*. We will show this procedure in the case in which all the factors have the same number of levels s , S prime, but it can also be applied to the general case. In Section 4 we have shown that counting functions must satisfy the following set of linear

equations

$$AY = \lambda \underline{1}$$

where A corresponds to the set of conditions \mathcal{C} written in terms of strata.

It follows that if, given a \mathcal{C} -compatible solution Y , such that $AY = \lambda \underline{1}$, we search for an additive move X such that $A(Y + X)$ is still equal to $\lambda \underline{1}$, we have to solve the following linear homogenous system

$$AX = 0$$

with $X = (x_\zeta), \zeta \in \mathcal{D}$, $x_\zeta \in \mathbb{Z}$ and $y_\zeta + x_\zeta \geq 0$ for all $\zeta \in \mathcal{D}$. We observe that this set of conditions allows to determine new \mathcal{C} -compatible solutions *that give the same λ* . We know that $\lambda = \frac{\# \mathcal{F}}{s}$ so this homogenous system determines moves that *do not change the dimension of the solutions*.

Let's now consider the extended homogeneous system, where \tilde{A} has already been defined in Section 4,

$$\tilde{A}\tilde{X} = 0$$

with $\tilde{X} = (\tilde{x}_\zeta), \zeta \in \mathcal{D}$, $\tilde{x}_\zeta \in \mathbb{Z}$ and $\tilde{y}_\zeta + \tilde{x}_\zeta \geq 0$ for all $\zeta \in \mathcal{D}$.

Given $\tilde{Y} = (Y, \lambda_Y)$, where Y is \mathcal{C} -compatible counting function and $\lambda_Y = \frac{\sum_\zeta y_\zeta}{s}$, the solutions of $\tilde{A}\tilde{X} = 0$ determine all the other $\tilde{Y} + \tilde{X} = (Y + X, \lambda_{Y+X})$ such that $\tilde{A}(\tilde{Y} + \tilde{X}) = 0$. $Y + X$ are \mathcal{C} -compatible counting functions whose sizes, $s\lambda_{Y+X}$, are, in general, *different from that of Y* .

5.1 Markov Basis

We use the theory of Markov basis (see for example Drton et al. (2009) where it is also available a rich bibliography on this subject) to determine a set of generators of the moves.

We use the following procedure in order to randomly select a \mathcal{C} -compatible counting function. We compute a Markov basis of $\ker(A)$ using 4ti2 (4ti2 team (2007)). Once we have determined the Markov basis of $\ker(A)$, we make a random walk on the *fiber* of Y , where Y , as usual, contains the values of the counting function of an initial design \mathcal{F} . The fiber is made by all the \mathcal{C} -compatible counting functions that have the same size of \mathcal{F} . The random walk is done randomly choosing one move among the feasible ones, i.e. among the moves for which we do not get negative values for the new counting function.

In the next paragraphs we consider moves for the cases that we have already studied in Section 4.

5.2 Orthogonal arrays

5.2.1 $OA(n, 2^5, 2)$

We use the matrix A , already built in Section 4.1.1 and give it as input to 4ti2 to obtain the Markov Basis, that we denote by \mathcal{M} . It contains 5.538 different moves. Given $M = (x_\zeta) \in \mathcal{M}$ we define $M^+ = \max(x_\zeta, 0)$ and $M^- = \max(-x_\zeta, 0)$. We have $M = M^+ - M^-$.

As an initial fraction \mathcal{F}_0 , we consider the eight-run regular fraction whose indicator function R_0 is

$$R_0 = \frac{1}{4}(1 + X_1 X_2 X_3)(1 + X_1 X_4 X_5)$$

We obtain the set of feasible moves observing that a move $M \in \mathcal{M}$, to be feasible, should be not negative when R_0 is equal to zero that means

$$(1 - R_0)M^- = 0$$

We find 12 moves. Analogously an element $M \in \mathcal{M}$ such that

$$(1 - R_0)M^+ = 0$$

gives a feasible move, $-M$. In this case we do not find any of such element.

Therefore, given R_0 , the set of feasible moves becomes \mathcal{M}_{R_0} that contains $12 + 0$ different moves.

We randomly choose one move M_{R_0} out of the 12 available ones and move to

$$R_1 = R_0 + M_{R_0}$$

We run 1.000 simulations repeating the same loop, generating R_i as $R_i = R_{i-1} + M_{R_{i-1}}$.

We obtain all the 60 different 8-run fractions, each one with 8 different points as in Carlini and Pistone (2007).

Using \tilde{A} we obtain the set $\tilde{\mathcal{M}}$ that contains 18 different moves.

5.2.2 $OA(n, 3^3, 2)$

Using A as built in the Section 4.1.2, we use 4ti2 to generate the Markov basis corresponding to the homogeneous system $AX = 0$. We obtain \mathcal{M} that contains 81 different moves.

As an initial fraction we can consider the nine-run regular fraction \mathcal{F}_0 whose indicator function R_0 is

$$R_0 = \frac{1}{3}(1 + X_1X_2X_3 + X_1^2X_2^2X_3^2)$$

We run 1.000 simulations repeating the same loop, i.e. generating R_i as $R_i = R_{i-1} + M_{R_{i-1}}$.

We obtain all the 12 different 9-run fractions, each one with 9 different points as known in the literature and as found in Section 4.1.2.

Using \tilde{A} we also obtain the set $\tilde{\mathcal{M}}$ that contains 10 different moves.

5.2.3 4×4 sudoku

Using the matrix A built in Section 4.3.1, we run 4ti2 getting the Markov basis \mathcal{M} that contains 34.920 moves.

We randomly choose an initial sudoku

| | | | |
|---|---|---|---|
| 3 | 2 | 4 | 1 |
| 4 | 1 | 3 | 2 |
| 2 | 3 | 1 | 4 |
| 1 | 4 | 2 | 3 |

The corresponding indicator function is

$$F_0 = \frac{1}{4}(1 - R_2C_1S_1S_2)(1 - R_1C_2S_1) .$$

Then we extract from \mathcal{M} the feasible moves. We obtain a subset \mathcal{M}_{F_0} that contains 5 different moves. We repeat the procedure on $-\mathcal{M}$ and we obtain other 9 moves.

We randomly choose one move M_{F_0} out of the $5 + 9$ available ones and move to

$$F_1 = F_0 + M_{F_0}$$

We run 1.000 simulations repeating the same loop $F_i = F_{i-1} + M_{F_{i-1}}$.

We obtained all the 288 different 4×4 sudoku.

6 Conclusions

We considered mixed level fractional factorial designs. Given the counting function R of a fraction \mathcal{F} we translated the constraint $c_\alpha = 0$, where c_α is a generic coefficient of its polynomial representation $R = \sum_\alpha c_\alpha X^\alpha$, into a set of linear constraints with integer coefficients on the values y_ζ that R takes on all the points $\zeta \in \mathcal{D}$. We obtained the set of generators of the solutions of some problems using Hilbert Basis. We also studied the moves between fractions. We characterized these moves as the solution of a homogeneous linear system. We defined a procedure to randomly walk among the solutions that is based on the Markov basis of this system. We showed the procedure on some examples. Computations have been made using 4ti2 (4ti2 team (2007)).

Main advantages of the procedure are that we do not put restrictions on the number of levels of factors and that it is not necessary to use software that deals with complex polynomials.

One limit is in the high computational effort that is required. In particular only a small part of the Markov basis is used because of the requirement that counting functions can only take values greater than or equal to zero. The possibility to generate only the moves that are feasible could make the entire process more efficient and is part of current research.

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